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Theoretical Study for the Effect of Pt Nanoparticles on Strontium Cerate and Zirconate

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Abstract

Trivalent-cation-doped $SrCeO_{3-\delta}$ and $SrZrO_{3-\delta}$ have protonic conductivity at intermediate temperatures. Recently, it has been reported that $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$ has higher conductivity than $SrZr_{0.9}Y_{0.1}O_{3-\delta}$ in H_2 after Pt nanoparticles precipitate. This study hypothesizes the precipitated Pt provides electrons for $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$ or $SrZr_{0.9}Y_{0.1}O_{3-\delta}$ However, density functional theory showed both $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$ and $SrZr_{0.9}Y_{0.1}O_{3-\delta}$ provide electrons for Pt.

1. Introduction

Proton conducting material have been widely investigated because of the potential as electrolytes for intermediate temperature solid oxide fuel cells. Recently, it has been reported that Pt dissolving in $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$ has higher conductivity than Pt dissolved in $SrZr_{0.9}Y_{0.1}O_{3-\delta}$ in H_2[1]. For the explanation of phenomena, this study hypothesizes the precipitated Pt provides electrons for $SrCe_{0.95}Yb_{0.05}O_{3-\delta}$ or $SrZr_{0.9}Y_{0.1}O_{3-\delta}$ To investigate the hypothesis, density functional theory was applied to the heterointerface between Pt and Yb-doped strontium cerate / Y-doped strontium zirconate.

2. Calculation

The bulk calculations of Pt-$Sr_8Zr_6M_2O_{23}$ and Pt-$Sr_8Ce_6M_2O_{23}$ (M = Y or Yb) was optimized. 500eV cutoff energy and 5×5×1 Monkhorst–Pack k-points were employed. In addition, to obtain the work function of $Sr_8Ce_6Y_2O_{23}$, each local potential in vacuum slab was investigated. 500eV cutoff energy and 3×4×1 Monkhorst–Pack k-points were employed.

3. Results

Figure1 and 2 show the optimized hetero interface between Pt and Y-doped $Sr_8Ce_6Yb_2O_{23}$ / $Sr_8Zr_6Yb_2O_{23}$. With these heterointerface, the results of charge transfer showed that Pt provided electrons for hydrated $Sr_8Ce_6Y_2O_{23}$, although platinum provided electrons for hydrated/dehydrated $Sr_8Zr_6Y_2O_{23}$. In the poster session, the reason of above phenomena will be discussed.

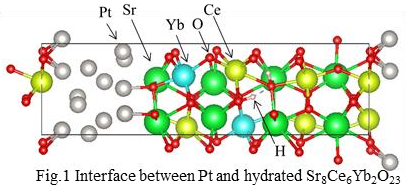

Fig.1 Interface between Pt and hydrated $Sr_8Ce_6Yb_2O_{23}$

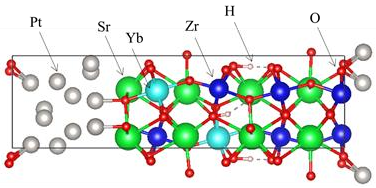

Fig.2 Interface between Pt and hydrated $Sr_8Zr_6Yb_2O_{23}$

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Reference

[1] Y. Takamura, *et al.*, (2016PRiME 2016, Honolulu, HI, U.S.A.

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